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MAGNETIC STRUCTURES AND PHASE TRANSFORMATIONS IN Mn-BASED CuAu-I TYPE ALLOYS

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BUDAPEST

Abstract

Investigations of the magnetic properties in the ordered CuAu-I-type manganese alloys are reviewed. The formation of the ordered phase and the possible magnetic structures are discussed. New experimental results for the Mn-Ni, Mn-Pd and Mn-Pt systems are reported.

Neutron diffraction shows the basic antiferromagnetic structure to be the same for all the alloys investigated. In MnPt a magnetic structure transformation has been observed. Below 800°K the magnetic moments turn from the basal plane gradually to the tetragonal axis. The variation of the transition temperature in the Mn-Pt system as well as that of the Néel temperature in the Mn-Ni, Mn-Pd and Mn-Pt systems with concentration were measured and are theoretically analyzed.

The dependence of lattice parameters on concentration and temperature was determined. The lattice parameters suffer a significant but continuous change near the Néel temperature which is attributed to Mn-Mn exchange interaction.

Magnetic susceptibility measurements support the neutron diffraction results. The increase in susceptibility, observed by several authors at lower temperatures, is found to be a result of contaminations.

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I. Introduction

The last decade has witnessed an ever growing interest in the antiferromagnetic behaviour of metals. Though, it was suggested by Néel [1] as early as 1932 that chromium and manganese had to be considered as antiferromagnetic, this assumption could not overrule the quite generally accepted conception of Kramers [2] that no antiferromagnetic structure can form in the metals. It was only in 1953 that the neutron diffraction experiments of Shull and Wilkinson [3] proved Néel's idea to be true by showing an antiferromagnetic order in chromium and α -manganese.

Among the four modifications of manganese the α and β modifications have very complex unit cells containing 58 and 20 atoms, respectively. Their magnetic structure is still imperfectly known. Neutron diffraction measurements [4] show that localized moments exist in α -manganese. In the β type, if any magnetic order occurs at all, the average value of the localized moments cannot exceed 0,5 μ_B . The structure of the high temperature fcc γ -phase was established indirectly in disordered Mn-rich Mn-Cu alloys by extrapolation to zero copper concentration [5, 6] . Practically nothing is known about the magnetic properties of δ -manganese stable at very high temperatures.

Thus the study of the interaction between the Mn atoms in chemically ordered Mn-alloys may help in contributing to the better understanding of the nature of antiferromagnetism in metals. That is why the ordered

MnMe and Mn_3Me-type alloys have been chosen for the investigations from which the experiments on MnMe will be reported in the present while those on Mn_3Me in another paper [7] .

Manganese forms homogeneous alloys with nickel, rhodium, palladium, iridium, platinum in the equiatomic concentration range. These alloys are of face-centered cubic at higher but of CuAu-I-type tetragonal structure at lower temperatures. In the CuAu-I phase all of these alloys are antiferromagnetic and the lattice parameters show anomalous dependence on both the concentration and temperature. In the antiferromagnetic state only the Mn atoms are likely to have any magnetic moment. Assuming a dependence of the magnetic interactions on the interatomic distances, a strong correlation is expected to exist between the anomalous behaviour of the lattice parameter and the magnetic order.

In paragraph II the formation and stability of the CuAu-I-type lattice, in III the possible magnetic structures will be discussed. In IV the experimental methods, while in V, VI and VII the results of the susceptibility, neutron and x-ray diffraction measurements will be reported and finally in VIII the conclusions will be presented.

II. CuAu-I-type Lattice

The CuAu-I-type crystal lattice is illustrated in Fig. 1. The structure can be characterized by two types of unit cell: the one a strongly distorted CsCl-type, containing two atoms, with parameters a_o, c_o, the other having four atoms, with parameters $a = \sqrt{2}a_o$, $c = c_o$. In the present paper the latter will be used.

The CuAu-I structure is very common among the alloys of equiatomic concentration [8] and stable over wide ranges of composition and temperature [9] . Manganese forms this type of alloy with nickel at 42-53, with palladium at 36-52, with iridium at 45-63, with platinum at 33-60 [9] and with rhodium at 50-65 [10, 11] atomic percent Mn concentration.

The Cu-Au-I structure usually results from the face-centered cubic phase [9] by an ordering transformation. In Mn-alloys, however, it is derived from an already ordered CsCl-type cubic phase with a marked distortion of the lattice. According to our neutron diffraction measurements [12] this is true also for MnNi in contrast with the observation of Coles and Hume-Rothery [13] . The transformation from CsCl to CuAu-I lattice was found for MnRh [10, 14] and MnNi [12] to be a diffusionless martensitic process and that is expected to hold also for the other Mn-alloys of this group.

In the Mn-alloys of non-stoichiometric composition the excess atoms generally occupy the positions in the sublattice of the other component at random. A secondary order with a doubled unit cell, resulting from the ordering of excess Pd atoms, could be, however, observed in the Mn-Pd system at about 40 at. % Mn concentration [15] .

III. Possible Magnetic Structures of the CuAu-I Lattice

Using some simple assumptions one can find the possible magnetic structures of the tetragonal CuAu-I lattice and interpret the experimental data by comparison with these structures. In Fig. 1 the Mn atoms are represented by empty, the Me atoms by full circles. If only the manganese atoms are assumed to have any magnetic moment, the possible structures can be derived by relatively simple calculation. Taking into account three interactions between the Mn atoms marked in Fig. 1 and using the molecular field approximation we get the structures listed in Table I.

In the case, when $U<0$ while $|U|>|V|$ and $|U|>|W|$ the structure can be only antiferromagnetic. Since the chemical and magnetic unit cells of the investigated alloys are identical, only model 3 of Table I. is allowed. The direction of the magnetic moments to the crystallographic axes is, however, still indefinite.

Assuming, in addition, that the antiferromagnetic structure results from the paramagnetic phase by a second order transition, it is possible to make some inferences on the directions and relative magnitudes of magnetic moments.

Using the Landau theory [16] we can determine the allowed directions of the moments for model 3. It turns out that only three structures, shown in Fig. 2 are possible. If the manganese moments are parallel to the tetragonal axis /model A in Fig. 2/ μ_{Me} must be zero, whereas with the moments lying in the basal plane the structures B or C with non-zero μ_{Me} are possible. Since the effective exchange field is zero at the Me-sites, the magnetic moment of Me atoms, if it is non-zero at all, can be due only to the much weaker anisotropic interaction of relativistic origin and must be therefore very small, thus the assumption $\mu_{Me} \sim 0$ is justified.

It may be noted that only two of the structures suggested by Kasper and Kouvel [17] , namely, those given by the authors under a/ and b/ are allowed by group theoretical considerations.

IV. Experimental

The magnetic properties of CuAu-I type Mn alloys were investigated on the systems Mn-Ni, Mn-Pd and Mn-Pt near the equiatomic concentration by magnetic susceptibility, neutron and x-ray diffraction measurements.

The samples were prepared by alloying metals of 99,9 percent purity in an induction furnace under argon atmosphere and homogenizing at 800 °C for 24 hours. The results of the chemical analysis are given for each sample in Table II. For the susceptibility measurements bulk, for the diffraction experiments powdered samples were used.

The susceptibility measurements were made with magnetic balance in the temperature range from liquid nitrogen temperature up to 800°C. The samples for the high temperature experiments were sealed in quartz ampoules at a pressure of 10^{-4} mmHg. The neutron diffraction measurements were carried out by an automatic neutron diffractometer at the VVRS reactor in Budapest, with neutrons of 1,15 Å wavelength from liquid helium temperature up to 800°C at 10^{-4} mmHg pressure. For the room temperature x-ray diffraction studies a Debye-Scherrer camera was used, while for high temperatures, up to 900°C, a furnace filled with 30 % H_2 and 70 % N_2 gas mixture and mounted on a Philips diffractometer was applied.

V. Susceptibility Measurements

The susceptibility data reported on the CuAu-I type Mn alloys are contradictory. In a Mn-Ni alloy of about equiatomic composition a temperature independent, low susceptibility was observed by Kasper and Kouvel [17] between 4,2° and 300°K. In contrast with this, Pearson et al. [18] observed the appearance of ferromagnetism in Mn-Ni with 45-53 at. % Mn concentrations at temperatures below 90°K and also an increase in the susceptibility in the temperature range from 300° to 600°K for specimens with 45-51 at. % Mn concentrations. This last effect, however, could not be observed on quenching from 640°C. A similar thermal behaviour of the susceptibility was found by Pearson et al. in Mn-Pt [19] and in Mn-Ir [20] alloys, too. In Mn-Pt alloys Yokoyama and Wuttig [21] observed the formation of a ferromagnetic oxide in the presence of oxygen and established its composition and structure as Mn_2Pt_2O of the cubic Fe_4N type. In Mn-Pd alloys in the concentration range from 34 to 42 at. % Mn the susceptibility increases during the annealing at temperatures between 400° and 500°C [15, 22, 23] . This was explained by the onset of a secondary order of the excess Pd atoms in the Mn sublattice. The appearance of a temperature independent susceptibility of MnRh alloy at low temperature was also reported [14] .

Considering these experimental data the question arises whether the observed magnetic behaviour might not be due to the presence of impurities. For this reason great care was taken in our investigations to keep the samples free from any contamination. The susceptibility vs. temperature curves for MnNi, MnPt and MnPd of stoichiometric composition, measured on both heating and cooling in the temperature range from 20° to 800°C, are shown in Fig. 3. Apart from the hysteresis apparent in Mn-Ni and Mn-Pd at high temperature, the curves are the same on both heating and cooling. The susceptibility remains low even at liquid nitrogen temperature in contrast with the data of Pearson et al. [18, 19] but repeating the measurement for MnNi at 10^{-2} mmHg pressure an appreciable increase in susceptibility, shown by the dashed line in Fig. 3, could be observed on cooling. This observation shows that the reported increase in susceptibility must be due to impurities the nature of which is not revealed by this measurement but, considering the phase diagrams in Ref. 9, they are undoubtedly formed in the CuAu-I phase. The lines separating the CuAu-I and CsCl phases shift towards higher temperatures with decreasing Mn concentration for both the Mn-Ni and the Mn-Pt systems, and attain the temperatures from which Pearson et al. quenched their Mn-Ni /640°C/ and Mn-Pt /950°C/ samples at about the equiatomic concentration. This means that at the annealing temperature only samples with less than equiatomic Mn-content had been in the CuAu-I phase and only these exhibited the increase in susceptibility at about 600°K in the measurements of Pearson et al. In the Mn-Pt alloys the impurity being formed is certainly the ferromagnetic oxide identified by Yokoyama and Wuttig [21] , which can form only in the CuAu-I phase.

The low value and the character of the temperature dependence of the susceptibility in Fig. 3 point to antiferromagnetism but no maximum associated with the Néel point can be seen. In MnPt and MnPd, however, the Néel temperature can be inferred from the break in the susceptibility curve. The hysteresis occurring in MnNi and MnPd at high temperatures shows the first-order transition into the CsCl phase.

The alloys of non-stoichiometric composition yield the same susceptibility curves as shown in Fig. 3 for runs at 10^{-4} mmHg pressure.

VI. Magnetic Structure Investigations

Studies of magnetic structure by powder neutron diffraction technique have been already reported on stoichiometric MnNi [17] , MnPd [16] and Mn_2Pd_3 [15 , 24] as well as on Mn-Pt alloys of various concentrations [25]. In each case the magnetic and atomic unit cells, except for Mn_2Pd_3 with

secondary order, were found to be identical, the structure to be pure antiferromagnetic in agreement with our susceptibility measurements. The spin arrangement was found to be of either the *B* or *C* type illustrated in Fig. 2, except for MnPt and $Mn_{1,1}Pt_{0,9}$ which have structure *A*, though in the former it transforms to *B* as the temperature increases [26].

Our neutron diffraction studies covered the magnetic structures and the transformations from liquid helium temperature up to 800°C.

The reflections from CuAu-I structure can be divided into two groups, namely, the basic nuclear reflections with unmixed h, k, l and the nuclear superreflections associated with the atomic order, with mixed h, k, l and h + k = 2n. Any of the antiferromagnetic structures *A*, *B* and *C* produces additional reflections with mixed h, k, l but h + k = 2n + 1. The relative intensities of the magnetic reflections depend on the angle φ_c between the magnetic moment and the crystallographic axis *c*. So e.g. the integrated intensity ratio of reflections (100) to (101) is 4:1 for structure *A* /Fig. 4a/ and 1:1 for structures *B* and *C* /Fig. 4b/. Of course the structures *B* and *C* cannot be distinguished using powdered samples but it is easy to see the difference between *A* and the other two.

It has been seen from the available experimental data and from the previous considerations that only Mn has appreciable magnetic moment [16, 17, 25, 26]. The values of the magnetic moment measured at room temperature and evaluated using the experimental form factor of Corliss et al. [27] are listed in Table II. It is seen that they do not vary substantially over the alloys investigated.

The magnetic transformations can be observed from the temperature behaviour of the magnetic reflections. A simultaneous observation of the nuclear reflections is needed if one wants to follow up any change in the order or in the structure of the crystal lattice. The Mn-Pt alloys with equiatomic or higher Mn concentration have the structure *A* at room temperature or lower. The Mn-Ni and Mn-Pd alloys are of either *B* or *C* structure from liquid helium temperature up to the Néel point.

The temperature variation of the (100) reflections for stoichiometric MnNi, MnPd and MnPt is shown in Fig. 5. For MnPd the (100)intensity shows a Brillouin-like dependence up to the Néel temperature. This is the case for MnNi up to 670°C where the reflection abruptly disappears together with the nuclear reflections from the CuAu-I structure. This disappearance is due to the transformation of the crystal lattice to the paramagnetic CsCl-structure. The Néel temperature of the antiferromagnetic phase can be estimated only by extrapolation /see dashed line in Fig. 5./.

For MnPt a well-marked variation of the intensity between 300° and 500°C indicates the transition from A to B structure, while the disappearance of this reflection permits to evaluate the Néel temperature of the latter. The $A \rightleftharpoons B$ transformation is clearly indicated by Fig. 4c showing the variation of the (100) and (101) reflections simultaneously.

The non-stoichiometric alloys show similar intensity variations. In Mn-Ni alloys a true Néel point is found only in $Mn_{0,91}Ni_{1,09}$. For the two other Mn-Ni samples it is evaluated by extrapolation since the allotropic transformation occurs already below the Néel temperature. In the Mn-Pt alloys the $A \rightleftharpoons B$ transformation is observable only in a narrow concentration range but it takes place over a wide range of temperature. Therefore the centre of this interval was chosen as the transformation temperature.

The values of the Néel point T_N and the temperatures T_s of the $A \rightleftharpoons B$ transformation are listed in Table II.

VII. Lattice Parameter Measurements

The variation of the lattice parameters with concentration has been already studied by Pearson et al. [18-20] who observed the parameter a to have a maximum, the parameter c a minimum at the stoichiometric concentration in Mn-Ni, Mn-Pt and Mn-Ir. Their explanation of this result by size effect due to the difference between the atomic radii, presents difficulties in the case of Mn-Ni. Our early investigations [16] have already shown a correlation between the magnetic interactions and the values of the lattice parameter.

The temperature dependence of the lattice parameters was studied by x-ray diffraction techique. The results for stoichiometric MnNi, MnPd and MnPt are shown in Fig. 6. A common feature of these curves is a strong contraction of a with a simultaneous and similarly strong dilatation of c on cooling below the Néel temperature from the paramagnetic state. This means that the dominant interaction determining the magnetic structure, presumably the nearest neighbour antiferromagnetic interaction, is strongly dependent on the interatomic distance and increases as the nearest neighbours get closer to each other.

The $A \rightleftharpoons B$ transformation of the magnetic structure does not affect the temperature dependence of the lattice parameters.

The curves obtained for the non-stoichiometric alloys are quite similar to those shown in Fig. 6. No difference can be observed in the

temperature dependence of the lattice parameters for samples of *A* or *B* structure.

The anomalous dependence of the lattice parameters on temperature can be satisfactorily explained if one assumes the effective interaction between nearest neighbour Mn-atoms to be more sensitive to the variation of the interatomic distance than that between next nearest neighbours. Let us characterize the dependence on the interatomic distance for the two types of interaction by parameters

$$\alpha = \left[\frac{dJ_1(\Delta)}{d\Delta}\right]_{\Delta=\frac{1}{\sqrt{2}}a_d} \quad \text{and} \quad \beta = \left[\frac{dJ_2(\Delta)}{d\Delta}\right]_{\Delta=c_d}, \qquad (7.1)$$

where a_d and c_d are the equilibrium lattice parameters of the crystal in the absence of magnetic interactions. It can be shown by simple calculation that the appearance of magnetic order involves a change in the lattice parameters that can be expressed as

$$a = a_d - \ell_a M^2 \quad \text{and} \quad c = c_d + \ell_c M^2, \qquad (7.2)$$

where ℓ_a and ℓ_c contain the elastic constants of the crystal and the parameters α and β. For tetragonal lattice they will have the forms

$$\ell_a = \frac{1}{2} n a_d \frac{\alpha a_d^2 c_{33} + 2\beta c_d^2 c_{13}}{c_{33}(c_{11}+c_{12}) - 2c_{13}^2} \quad \text{and} \quad \ell_c = \frac{1}{2} n c_d \frac{\alpha a_d^2 c_{13} + 2\beta c_d^2 (c_{11}+c_{12})}{c_{33}(c_{11}+c_{12}) - 2c_{13}^2} \qquad (7.3)$$

where n is the number of Mn-atoms per unit volume and c_{ik} is the corresponding component of the elastic stiffness tensor.

Accepting Goodenough's [28] estimate for the dependence of Mn-Mn exchange interactions on interatomic distance, it can be assumed that $\alpha > 0$ and $\alpha > \beta$ hence $\ell_a > 0$ and $\ell_c > 0$. In this case the calculated values of the lattice parameters change with the temperature below the Néel point in the manner as observed. The change is mainly caused by the temperature dependence of the square of the sublattice magnetization per Mn-atom, since the temperature dependence of the quantities ℓ_a and ℓ_c is relatively slight.

The deformation sensitive magnetic interactions are expected to play an important role in the concentration dependence of the lattice parameters of the non-stoichiometric alloys, too. Assuming that the excess atoms are distributed over the sublattice of the other completely random it can be shown that the measured concentration dependence is predominantly magnetic in origin only if the requirement $\alpha' M_{Me} > \alpha M_{Mn}$ is fulfilled, where α' is a parameter for the Mn-Me interaction similar to α. Since

$M_{Me} \ll M_{Mn}$, we cannot expect this inequality to be fulfilled, the explanation must be attempted along other lines.

VIII. Summary

All of the investigated CuAu-I type Mn alloys have the same simple antiferromagnetic structure, differing only in the relative angles of the magnetic moments to the crystallographic c -axis. Only the Mn atom has appreciable magnetic moment and this does not vary essentially with the composition. If the magnetic moments of the Mn atoms are parallel to the c -axis, the other atoms cannot have any magnetic moment at all. In Mn-Pt alloys the magnetic moment is observed to turn gradually from parallel to normal with respect to the c -axis as the temperature increases from 300° to 500°C and this indicates a change in the character of the magnetic anisotropy. In the contamination free alloys neither ferro- nor ferrimagnetism is observed.

The anomalous temperature dependence of the lattice parameters can be explained in most cases by the effect of deformation sensitive nearest neighbour Mn-Mn interaction. The anomaly in the temperature dependence of the lattice parameters is proportional to the square of the sublattice magnetization. The sign of the proportionality factors is such that the transformation from the paramagnetic to the antiferromagnetic phase causes the a -axis to contract and the c -axis to dilate.

The lattice parameters exhibit extreme values /maximum for a , minimum for c / at the stoichiometric composition which, in addition to the deformation sensitive Mn-Mn and Mn-Me interactions, must be presumably due also to the deformation dependence of the ordering energy and to size effects.

The dominant interaction responsible for the antiferromagnetic structure is the nearest neighbour Mn-Mn interaction which increases with decreasing interatomic distance. The value of the Néel temperature for the stoichiometric alloys are consistent with this fact, since they increase when the distance between the nearest neighbour Mn atoms decrease. / T_N is highest in MnNi and lowest in MnPd/.

In the non-stoichiometric alloys the Néel temperature is lower than in the stoichiometric ones in spite of the decrease in the lattice parameter a with increasing deviation from the stoichiometric concentration.

This fact can be explained in the case of excess Mn atoms very simply since Mn atoms in the Me sublattice have as many nearest neighbours with antiparallel as with parallel moment. The next nearest neighbour Mn atoms, however, have always antiparallel moments which is energetically not favourable since the exchange interaction between them is certainly ferromagnetic. Therefore the presence of excess Mn atoms causes the Néel temperature to decrease if the ferromagnetic coupling of their next nearest neighbours is strong enough to overwhelm the effect of the decrease in the lattice parameter a .

The lower Néel temperature in the Mn deficient alloys can be explained by the ferromagnetic coupling of the nearest neighbour Mn-Me pairs, which predominates over the effect of the change in the parameter a.

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References

[1] L. Néel, Ann, Phys. /Paris/ 17, 64 /1932/

[2] H.A. Kramers, Physica 1, 182 /1934/

[3] C.G. Shull and M.K. Wilkinson, Rev. Mod. Phys. 25, 100 /1953/

[4] J.S. Kasper and B.W. Roberts, Phys. Rev. 101, 537 /1956/

[5] D. Meneghetti and S.S. Sidhu, Phys. Rev. 105, 130 /1957/

[6] G.E. Bacon, I.W.Dunmur, J.H. Smith and R.Street, Proc. Roy. Soc. A241, 223 /1957/

[7] E. Krén, P. Szabó, L. Pál, T. Tarnóczi, G. Kádár and C. Hargitai, J. Appl. Phys. /to be published/

[8] W. B. Pearson, Handbook of Lattice Spacings and Structures of Metals and Alloys, Pergamon Press, London, New York, 1958.

[9] M. Hansen, Constitution of Binary Alloys, McGraw-Hill, New York, 1958

[10] A. Kussmann, K. Müller and H. Wollenberger, Z. ang. Physik 20, 461 /1966/

[11] Y. Nakayama and M. Asanuma, Jap. J. Appl. Phys. 4, 315 /1965/

[12] E. Krén, E. Nagy, I. Nagy, L. Pál and P. Szabó, KFKI Report 10/1967

[13] B. R. Coles and W. Hume-Rothery, J. Inst. Metals 80, 85 /1951/

[14] J.S. Kouvel, C.C. Hartelius and L.M. Osika, J. Appl. Phys. 34, 1095 /1963/

[15] E. Krén, G. Kádár and T. Tarnóczi, Phys. Letters, 25A, 56 /1967/

[16] E. Krén and J. Sólyom, Phys. Letters 22, 273 /1966/

[17] J.S. Kasper and J.S. Kouvel, J. Phys. Chem. Solids 11, 231 /1959/

[18] W.B. Pearson, K. Brun and A. Kjekshus, Acta Chem. Scand. 19, 477 /1965/

[19] K. Brun, A. Kjekshus and W.B. Pearson, Phil. Mag. 10, 291 /1964/

[20] K. Brun, A. Kjekshus and W.B. Pearson, Acta Chem. Scand. 19, 107 /1965/

[21] T. Yokoyama and M. Wuttig, Z. Metallkunde 54, 308 /1963/

[22] R. Wendling, C.R. Acad. Sci. Paris 252, 408 /1961/

[23] H. Yamauchi, J. Phys. Soc. Japan 19, 652 /1964/

[24] J.A. Gonzalo and M.I. Kay, J. Phys. Soc. Japan 21, 1626 /1966/

[25] A.F. Andresen, A. Kjekshus, R. Møllerud and W.B. Pearson, Phil. Mag. 11, 1245 /1965/

[26] E. Krén, M. Cselik, G. Kádár and L. Pál, Phys. Letters 24A 198 /1967/

[27] L.M. Corliss, N. Elliott and J.M. Hastings, Phys. Rev. 104, 924 /1956/

[28] J.B. Goodenough, Magnetism and the Chemical Bond, Interscience, New York 1963.

Table I

No.	Configuration	Internal energy
1	$\bar{m}_1=\ldots=\bar{m}_8=\bar{m}$	-8U-4V-4W
2	$\bar{m}_1=\bar{m}_2=\bar{m}_3=\bar{m}_4=\bar{m}$ $\bar{m}_5=\bar{m}_6=\bar{m}_7=\bar{m}_8=-\bar{m}$	-8U+4V-4W
3	$\bar{m}_1=\bar{m}_2=\bar{m}_5=\bar{m}_6=\bar{m}$ $\bar{m}_3=\bar{m}_4=\bar{m}_7=\bar{m}_8=-\bar{m}$	8U-4V-4W
4	$\bar{m}_1=\bar{m}_2=\bar{m}_7=\bar{m}_8=\bar{m}$ $\bar{m}_3=\bar{m}_4=\bar{m}_5=\bar{m}_6=-\bar{m}$	8U+4V-4W
5	$\bar{m}_1=\bar{m}_3=\bar{m}_5=\bar{m}_7=\bar{m}$ $\bar{m}_2=\bar{m}_4=\bar{m}_6=\bar{m}_8=-\bar{m}$	-4V+4W
6	$\bar{m}_1=\bar{m}_3=\bar{m}_6=\bar{m}_8=\bar{m}$ $\bar{m}_2=\bar{m}_4=\bar{m}_5=\bar{m}_7=-\bar{m}$	4V+4W

Possible magnetic structures in CuAu-I-type lattice. $\underline{m}_1 \ldots\ldots \underline{m}_8$ are the unit vectors of the magnetic moments at different lattice sites of Fig. 1

$$U=\frac{1}{4}J_1 NM^2,\quad V=\frac{1}{4}J_2 NM^2,\quad W=\frac{1}{2}J_3 NM^2$$

where J_1, J_2 and J_3 are the effective exchange interaction constants, N is the number of Mn atoms in the crystal and M is the absolute value of the magnetic moment of Mn.

Table II.

Specimen	at% Mn	a(Å)	c(Å)	c/a	Magnetic structure type	$\mu_{Mn}(\mu_B)$	T_S (°C)	T_N (°C)
$Mn_{0,91}Ni_{1,09}$	45,4	3,72	3,54	0,952	B	3,8±0,3	-	760±30
MnNi	50,0	3,74	3,52	0,942	B	3,8±0,3	-	800±40
$Mn_{1,07}Ni_{0,93}$	53,4	3,74	3,53	0,845	B	3,7±0,3	-	740±40
$Mn_{0,90}Pt_{1,10}$	45,3	3,97	3,73	0,940	B	4,2±0,2	-	630±20
$Mn_{0,96}Pt_{1,04}$	48,0	3,99	3,67	0,920	B	4,2±0,2	< -268	680±10
MnPt	50,3	4,00	3,67	0,918	A	4,3±0,2	~ 440	700±10
$Mn_{1,04}Pt_{0,96}$	52,3	3,99	3,67	0,920	A	4,2±0,2	~ 510	610±20
$Mn_{1,13}Pt_{0,87}$	56,4	3,97	3,71	0,935	A	3,9±0,2	-	420±20
$Mn_{0,80}Pd_{1,20}$	40,1	4,05	3,64	0,899	B	4,2±0,2	-	340±10
$Mn_{0,88}Pd_{1,12}$	44,0	4,06	3,61	0,889	B	4,4±0,3	-	560±20
MnPd	50,0	4,07	3,58	0,880	B	4,4±0,4	-	540±10
$Mn_{1,03}Pd_{0,97}$	51,6	4,07	3,59	0,882	B	4,3±0,2	-	490±10

Crystal and magnetic structural data at room temperature, values of the transition temperature T_S and the Néel-pont T_N .

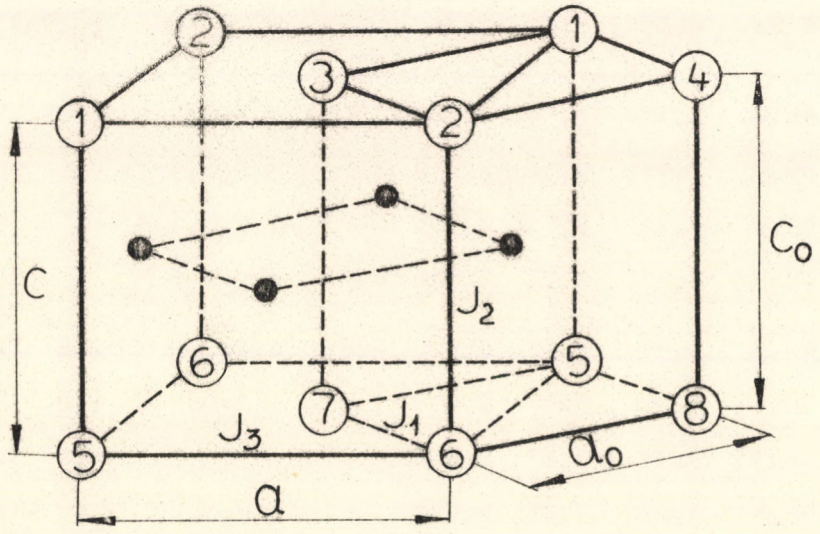

Fig. 1 Crystal lattice of Cu-Au-I-type. The Mn-sites are marked by numbers in circles. J_1, J_2 and J_3 show the assumed interactions

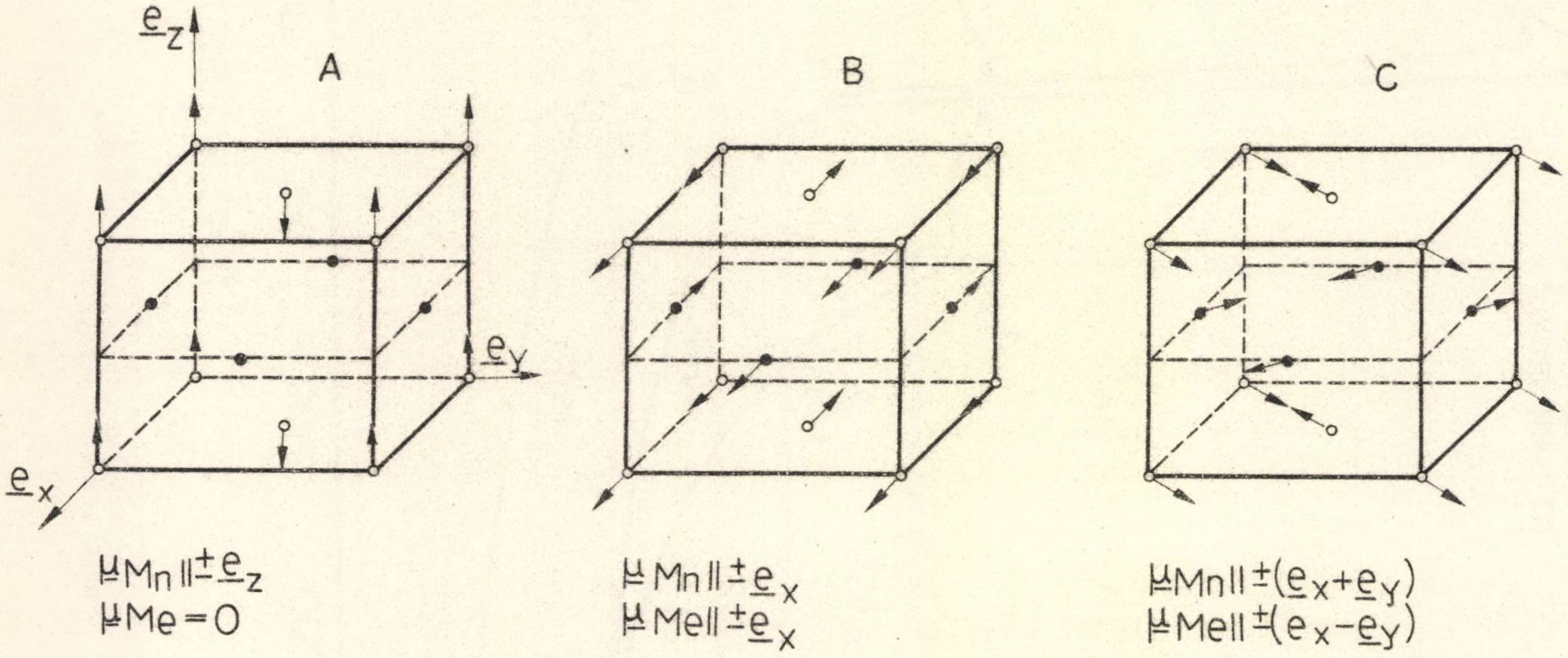

Fig. 2 Allowed magnetic structures in the Cu-Au-I lattice. The Mn and Me atoms are represented by empty and full circles, respectively

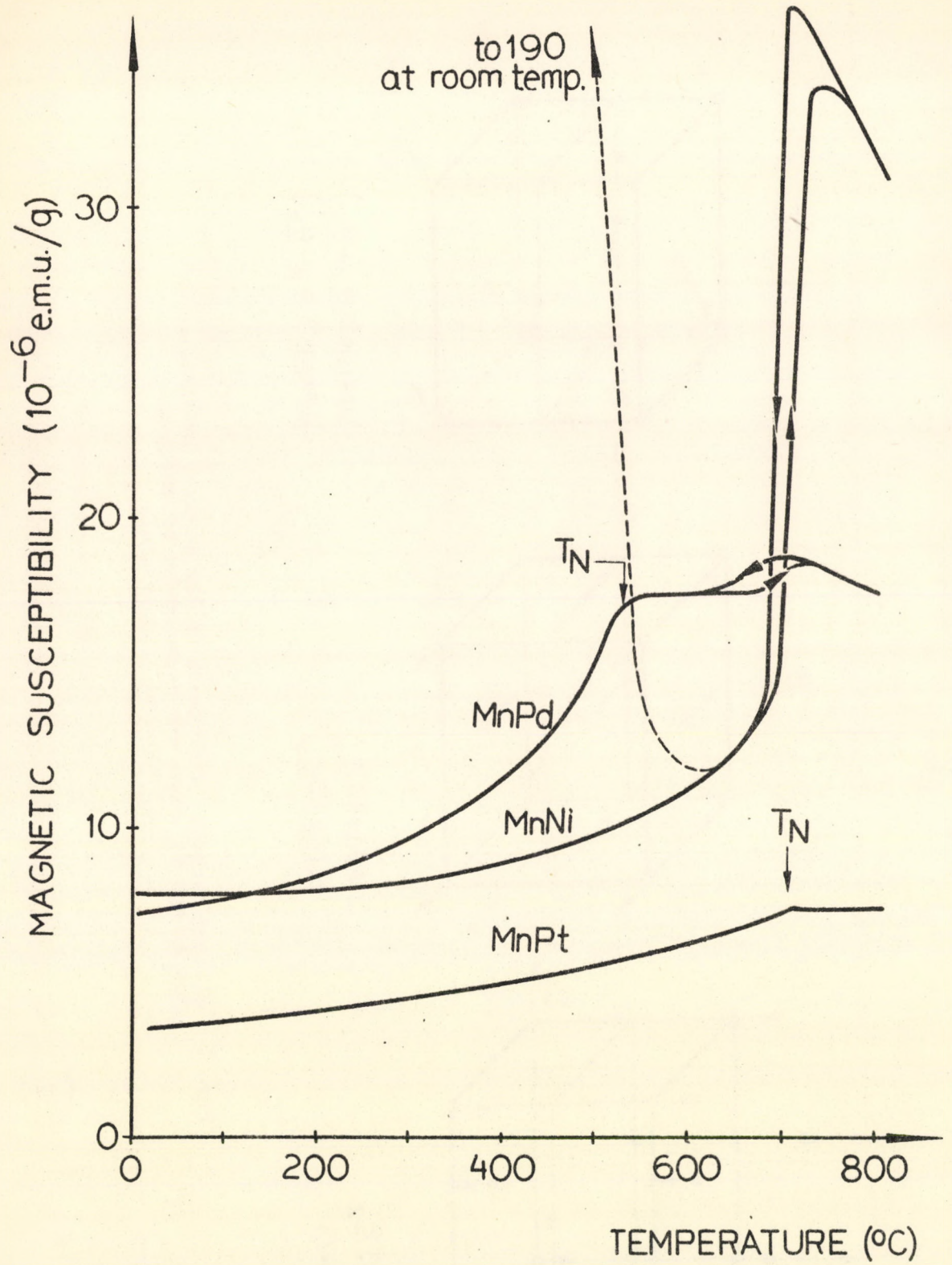

Fig. 3 Temperature dependence of the magnetic susceptibility for stoichiometric MnNi, MnPd and MnPt alloys

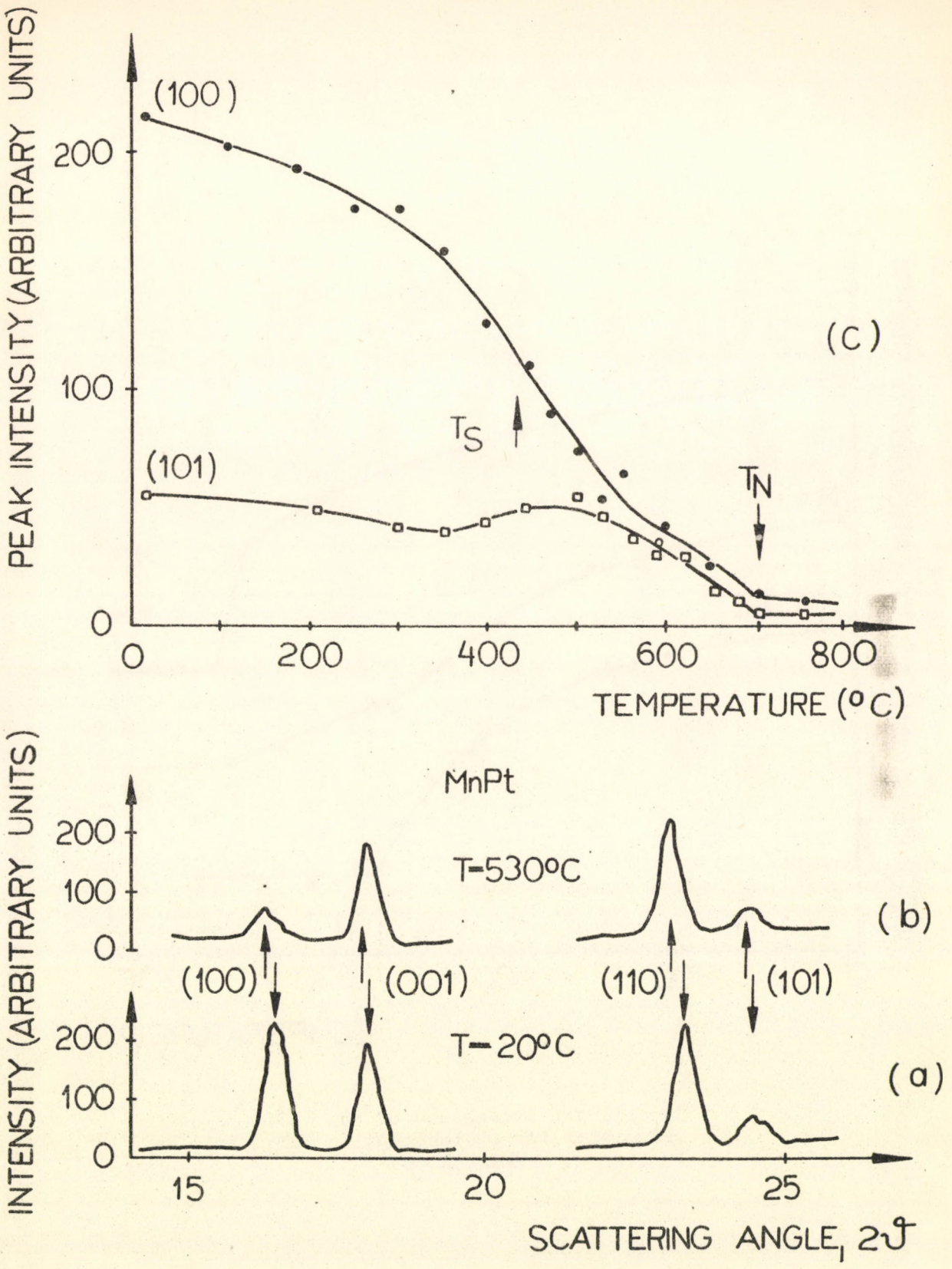

Fig. 4 Neutron diffraction results for MnPt. a/ Neutron diffraction pattern at 20°C. b/ Neutron diffraction pattern at 530°C. c/ Temperature dependence of the (100) and (101) magnetic reflections

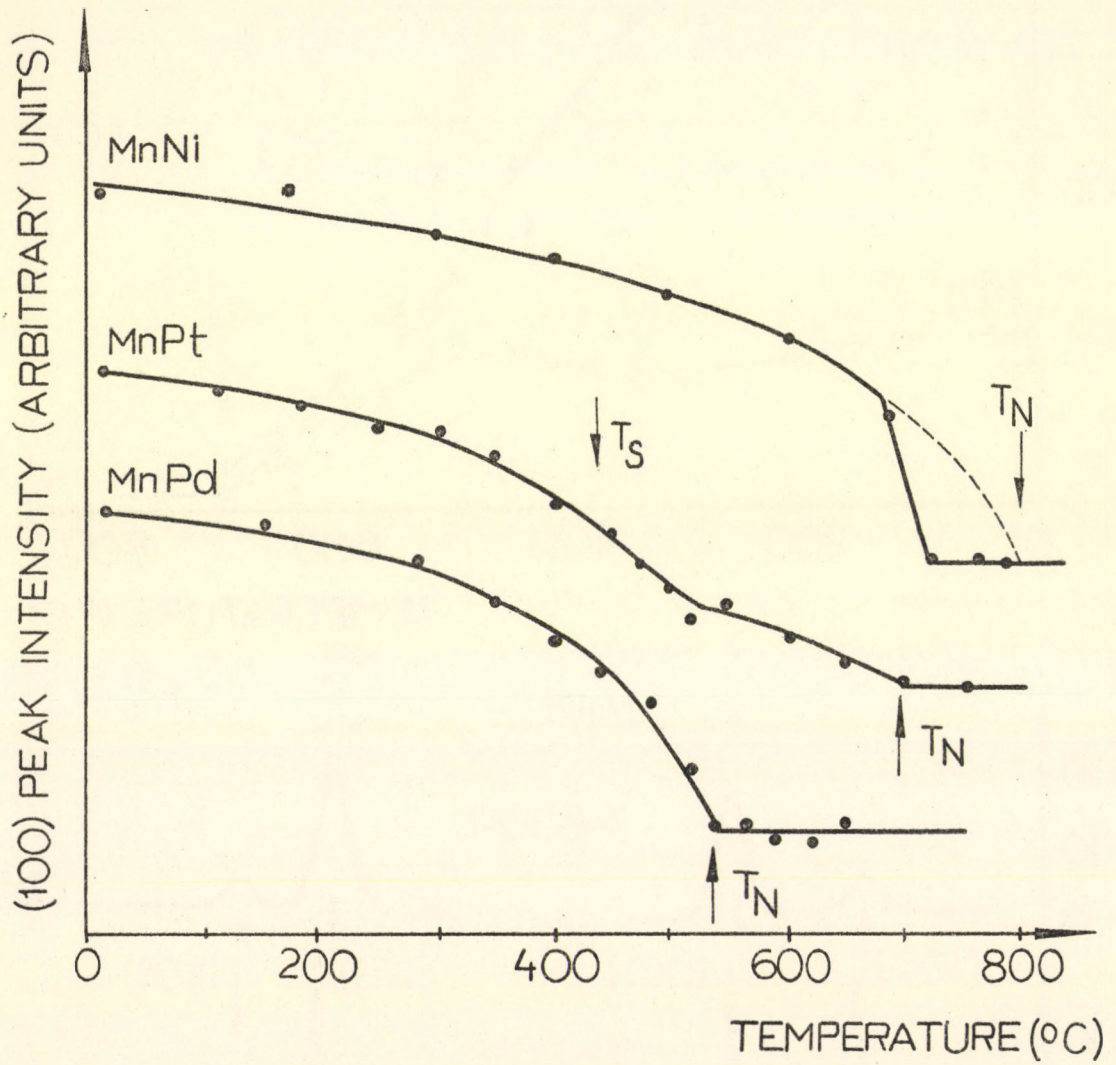

Fig. 5 Temperature dependence of the (100) magnetic reflection for stoichiometric MnNi, MnPd and MnPt alloys

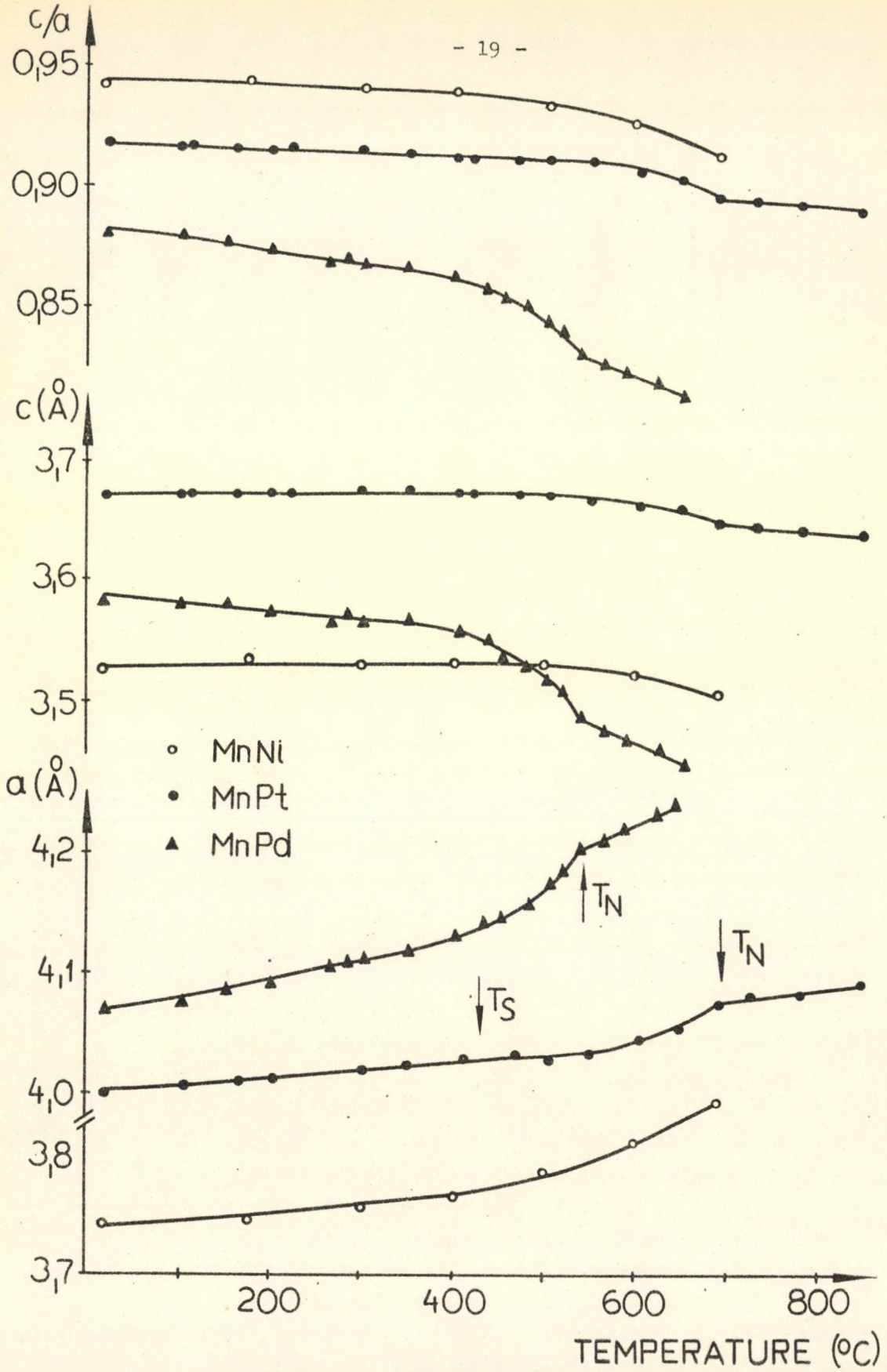

Fig. 6 Temperature dependence of the lattice parameters a and c for stoichiometric MnNi, MnPd and MnPt alloys

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